Physics – Uspekhi **52** (10) 977 – 988 (2009)

REVIEWS OF TOPICAL PROBLEMS PACS numbers: **74.20.–z**, 74.70.Ad, 74.78.Fk

Study of layered superconductors in the theory of an electron – phonon coupling mechanism

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DOI: 10.3367/UFNe.0179.200910a.1033

Contents

Abstract. We summarize a number of recent developments in the study of layered superconductors using the electron–phonon Eliashberg theory. The critical temperature of layered superconductors is calculated using the Eliashberg theory. The influence of nonadiabaticity effects on the critical temperature in layered superconductors is considered. The influence of Coulomb repulsion on the critical temperature is investigated in the case of an arbitrary thicknesses of conducting layers. Bardeen–Cooper–Schrieffer (BCS) equations for layered superconductors are used for the calculation of a specific heat jump, which is smaller than in the case of an isotropic BCS theory. The plasmon spectrum of layered superconductors with an arbitrary thicknesses of conducting layers is calculated. The influence of fluctuations in the order parameter phase on the critical temperature of layered superconductors is studied using the Ginzburg–Landau functional for the free energy. The results are shown to be in qualitative agreement with some experimental data for cuprate superconductors and recently discovered MgB_2.

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Received 5 December 2008, revised 18 June 2009
Uspekhi Fizicheskikh Nauk **179** (10) 1033 – 1045 (2009)
DOI: 10.3367/UFNr.0179.200910a.1033
Translated by I N Askerzade; edited by A M Semikhatov

1. Introduction

Twenty-three years after their discovery, cuprate high-temperature superconductors (HTSCs) [1] are still central topics of interest in physics. The mechanism of superconductivity is under lively debate [2, 3]. In [4], the isotope effect in the $Y_{1-x}Pr_xBaCu_3O_{7-\delta}$ compound [4] in all phases (superconducting, spin glass, and antiferromagnetic) was reported. For the high-T_c superconductors that have been of interest during the last decade, the experimental data in [5] suggests that the Fermi energy ranges between $E_F \sim 0.1-0.3$ eV and that the Debye phonon energy is of the order of $\omega_D \sim 0.08-0.16$ eV, making the ratio ω_D/E_F not negligible. Although somewhat debatable, there is experimental evidence [6] that electron–phonon interactions can be used to explain the fundamental mechanism operating in high-T_c superconductors. The existence of a strong electron–phonon interaction in cuprate superconductors was confirmed by the observation of a subgap structure in tunnel Josephson junction experiments [7]. As discussed in [8], similar phenomena occur due to the interaction of a Josephson current with phonons. As shown very recently in [9, 10], the electron–phonon mechanism explains many features of the low-energy relaxation process in cuprate superconductors, including the high values of the critical temperature. The structural element of HTSC compounds related to the location of mobile charge carriers is stacks of a certain number ($n = 1, 2, 3, \ldots$) of CuO_2 layers [11, 12]; there have been recent developments in growing SC/dielectric superlattices in which the thicknesses of the planes vary within a wide range. Variations in superlattice parameters, such as the thickness and the material of the layers, strongly influence the critical temperature.

The recent discovery of superconductivity in MgB_2 [13] has attracted a considerable attention. The magnesium diboride MgB_2 structure consists of an alternative stacking of the boron layer and the magnesium layer [14]. The

new materials are metallic and hence are promising as regards their application in various fields [15]. Several experiments indicate a phonon-mediated superconductivity mechanism in MgB_2 [16, 17]. The mass anisotropy parameter $\gamma = (m_c/m_{ab})^{1/2}$ of MgB_2 in the literature ranges from 1.2 to 9 in polycrystalline samples [14], and 4.31 to 4.6 in single crystals [18, 19]. It is well known that high-T_c superconductors evince a layered structure, related to CuO_2 layers or CuO_2 bilayers. The magnesium diboride MgB_2 is quite similar to cuprate superconductors, but with moderate anisotropy effects [18]. It is widely accepted that boron planes are conducting planes like the CuO_2 planes in cuprate superconductors [20].

The relatively high T_c value has motivated many studies, as has the observation that the detailed superconducting properties of MgB_2 significantly deviate from those calculated using the standard Bardeen–Cooper–Schrieffer (BCS) model. The two-band BCS theory taking the van Hove singularity of density of states into account was recently developed in [21]. It is well known that low-temperature superconductors are well described by the isotropic Eliashberg theory, with an isotropic electron–phonon spectral density $\alpha^2F(\omega)$ for the average interaction over the Fermi surface. This function is accurately known from inversion of tunneling data. In many cases, $\alpha^2F(\omega)$ has also been calculated from first-principle electronic band structure calculations extended to include the electron–phonon interaction, sometimes with the phonons taken directly from inelastic neutron scattering measurements. In many cases, such results agree very well with the corresponding tunneling data. In principle, the electron–phonon spectral density for the various electrons on the Fermi surface is anisotropic, leading to the energy gap anisotropy [22].

Theoretical calculations show that the MgB_2 Fermi surface has several pieces and is very anisotropic [23]. The electron–phonon interaction varies greatly on the Fermi surface [24, 25]. In [26], the superconducting transition temperature in MgB_2 was calculated using the *ab initio* pseudopotential density functional method in the framework of Eliashberg equations [27, 28]. Fully anisotropic Eliashberg equations in a strong-coupling regime were used in [26]. In contrast to previous works, the approach presented here is analytic, and we take the layered character of anisotropy in MgB_2 into account. The corresponding matrix elements for the electron–phonon and Coulomb interactions are taken from [29]. In recent works, the heat capacity anomaly at the transition to superconductivity of the layered superconductor MgB_2 has been compared to first-principle calculations with the Coulomb repulsion taken into account. The results obtained in the approach presented here also show that the conventional phonon-mediated electron pairing theory involving anisotropy effects can explain the origin of high T_c in magnesium diboride, MgB_2.

In this paper, we summarize recent research using the anisotropic Eliashberg theory and use it to determine the critical temperature of layered superconductors. The paper is organized as follows. In Section 2, we present the Eliashberg equations for layered superconductors, modified by taking nonadiabaticity effects into account. The specific heat jump of layered superconductors is calculated in the BCS model. At the end of that section, we study Coulomb effects and the plasmon spectrum of layered superconductors. The influence of order parameter fluctuations on the critical temperature is also considered in Section 2. Section 3 is devoted to results and their discussion. In Section 4, conclusions are made.

2. Basic equations of the electron–phonon theory

2.1 Eliashberg equations for layered systems

It is well known that the Eliashberg equations, which are the general equations of the electron–phonon theory, were first presented for isotropic superconductors by Eliashberg in the adiabatic limit [27]. In this limit, the nonadiabaticity parameter $m = \omega_D/E_F \ll 1$ is negligible. The isotropic equations can be written as

$$1 - Z(\omega) = -\frac{1}{\omega}\int_0^\infty d\omega'\,\lambda(\omega,\omega')\,, \tag{1}$$

$$Z(\omega)\Delta(\omega) = \int_0^\infty \frac{d\omega'}{\omega'}\tanh\frac{\omega'}{2T_c}\left[\lambda(\omega,\omega') - \mu\theta(E_F-\omega')\right]\mathrm{Re}\,\Delta(\omega')\,, \tag{2}$$

where $Z(\omega)$ is the electron mass renormalization parameter due to the electron–phonon interaction and $\Delta(\omega)$ is the energy gap. The electron–phonon coupling parameter $\lambda(\omega,\omega')$ can be expressed in terms of the electron–phonon spectral density function $\alpha^2F(\omega)$ [28]. In Eqn (2), $\mu\theta(E_F-\omega')$ is the Coulomb repulsion. In the case of layered systems, the strong anisotropy of the order parameter in directions perpendicular to the layers leads to the additional dependence $\Delta(p_z,\omega)$. We can then write the Eliashberg equations as [28]

$$1 - Z(p_z,\omega) = -\frac{1}{\omega}\int_0^\infty d\omega'\int_{-\pi}^{\pi}\frac{d(p_z'd)}{2\pi}\,\lambda_{p_z,p_z'}(\omega,\omega')\,, \tag{3}$$

$$Z(p_z,\omega)\Delta(p_z,\omega) = \int_{-\pi}^{\pi}\frac{dp_z'}{2\pi/d}\int_0^\infty\frac{d\omega'}{\omega'}\tanh\frac{\omega'}{2T_c} \times\left[\lambda_{p_z,p_z'}(\omega,\omega') - \mu_{p_z,p_z'}\theta(E_F-\omega')\right]\mathrm{Re}\,\Delta(p_z',\omega')\,, \tag{4}$$

where

$$\lambda_{p_z,p_z'}(\omega,\omega') = 2\int_0^\infty \alpha^2(\omega'')F_{p_z,p_z}(\omega'')\,K(\omega,\omega',\omega'')\omega''\,d\omega''\,, \tag{5}$$

$$K(\omega,\omega',\omega'') = \frac{1}{\omega+\omega'+\omega''+i\delta} + \frac{1}{-\omega+\omega'+\omega''-i\delta}\,.$$

In a layered system, we also take the anisotropic character of the Coulomb repulsion into account.

Because the magnesium diboride and cuprate compounds of recent interest consist of layered structures, we assume a dispersion relation appropriate for a layered system of the form [30–32]

$$E(\mathbf{k}) = \frac{\hbar^2(k_x^2+k_y^2)}{2m} + 2t\left[1-\cos(k_zd)\right], \tag{6}$$

where m is the in-plane effective mass, t is the transverse interlayer transfer matrix element (or tunneling integral), and d is the lattice constant in the z-direction. t characterizes the intensity of electron tunneling between the layers and must depend on the ratio d/b, $t = F(d/b)$, where b is a characteristic

distance of the order of the unit cell size in SC layers. The $F(d/b)$ function rapidly decreases as the distance d increases. It is possible, in principle, to obtain an explicit expression for this function if the electron density distribution inside the superconducting layers is known.

Such an energy spectrum of carriers was used in [33] (also see the references therein) for the calculation of various properties of layered superconductors. For $E > 4t$, the Fermi surface is open and the density of states $N(E)$ is constant. The phonon spectrum of the layered crystals is generally anisotropic. The dispersion relation for longitudinal $\omega_{\mathrm{L}}(q, q_z)$ and transverse $\omega_{\mathrm{T}}(q, q_z)$ phonons is given by

$$\omega_{\mathrm{L}}^2(q, q_z) = u_{\parallel}^2(q_x^2 + q_y^2) + 2\,\frac{u_z^2}{d}\left[1 - \cos(q_z d)\right], \tag{7}$$

$$\omega_{\mathrm{T}}^2(q, q_z) = u_z^2(q_x^2 + q_y^2) + 2\,\frac{u_{\mathrm{T}}^2}{d}\left[1 - \cos(q_z d)\right] \tag{8}$$

(the sound velocities satisfy the condition $u_{\parallel} \gg u_{\mathrm{T}}, u_z$). As mentioned in [34–36], the functions appearing in the generalized Eliashberg equations are defined by averaging over the Fermi surface. In the case of energy spectrum (6), this procedure is equivalent to the integration

$$\int_0^{2\pi} \mathrm{d}\phi \ldots = 4\int_0^{2p_0^*} \frac{\mathrm{d}q}{\left[(2p_0^*)^2 - q^2\right]^{1/2}} \ldots, \tag{9}$$

where $(p_0^*)^2 = p_0^2 - 4mt[1 - \cos(p_z d)]$ and ϕ denotes the angle between $\mathbf{p}$ and $\mathbf{p}'$, which is equal to p_0^*. It is clear that the region of phonon transfer momenta $q = 2p_0^*$ makes a major contribution to the integrals. By virtue of the last argument, the generalized Eliashberg equations for layered systems can be obtained from [30, 31] with the Einstein spectrum of the effective frequency ω_0, which is determined by the expression (see Section 2.2 for the phonon modes in layered systems)

$$\begin{aligned}
\omega_0 &= \sqrt{\omega_{\mathrm{av}}^2} \\
&= \left[\frac{d}{2\pi}\int_{-\pi/d}^{\pi/d} \mathrm{d}q_z\,\frac{2}{\pi}\,N_{2\mathrm{D}}\int_0^{2p_0^*} \frac{\mathrm{d}q}{\left[(2p_0^*)^2 - q^2\right]^{1/2}}\,\omega_{\mathrm{L}}^2(q, q_z)\right]^{1/2} \\
&\times \left[\frac{d}{2\pi}\int_{-\pi/d}^{\pi/d} \mathrm{d}q_z\,\frac{2}{\pi}\,N_{2\mathrm{D}}\int_0^{2p_0^*} \frac{\mathrm{d}q}{\left[(2p_0^*)^2 - q^2\right]^{1/2}}\right]^{-1/2} \\
&= \left[2u_{\parallel}^2(p_0^2 - 4mt) + \frac{2u_z^2}{d^2}\right]^{1/2}.
\end{aligned} \tag{10}$$

In the case of quasi-two-dimensional energy spectrum (6), Fermi-surface harmonics can be represented by $\cos(np_z d)$ [28]. The anisotropic electron–phonon coupling parameter $\lambda(p_z, p_z')$ is expanded as

$$\begin{aligned}
\lambda_{p_z, p_z'}(\omega, \omega') &= \lambda_{00}(\omega, \omega') + \lambda_{10}(\omega, \omega')\cos(p_z d) \\
&+ \lambda_{01}(\omega, \omega')\cos(p_z' d) + \lambda_{11}(\omega, \omega')\cos(p_z d - p_z' d),
\end{aligned} \tag{11}$$

where $\lambda_{ij}(\omega, \omega') = \lambda_{ij} I(\omega, \omega') = \lambda_{ij}\int \mathrm{d}\omega''\, K(\omega, \omega', \omega'')$.

As pointed out in [37, 38], the off-diagonal elements of the electron–phonon interaction in layered systems with electron spectrum (6) are proportional to t/E_{F}. Within the model of Fermi-surface harmonics, the order parameter takes the form

$$\Delta(p_z, \omega) = \Delta_0(\omega) + \Delta_1(\omega)\cos(p_z d). \tag{12}$$

With Eqn (11) taken into account, the expression for $Z(p_z, \omega)$ becomes

$$\begin{aligned}
Z(p_z, \omega) &= 1 + \lambda_{00}(\omega) + \lambda_{10}(\omega)\cos(p_z d) \\
&= Z_{00}(\omega) + \lambda_{10}(\omega)\cos(p_z d).
\end{aligned} \tag{13}$$

Substituting Eqns (12) and (13) in (3) and (4), we have the system of coupled integral equations

$$\begin{aligned}
&Z_{00}(\omega)\Delta_0(\omega) + \frac{\lambda_{10}(\omega)\Delta_0(\omega)}{2} \\
&\quad = \int_0^{\infty} \frac{\mathrm{d}\omega'}{\omega'}\tanh\frac{\omega'}{2T_{\mathrm{c}}}\,I(\omega, \omega')\lambda_{00}\Delta_0(\omega) - \varkappa_{00} \\
&\quad + \int_0^{\infty} \frac{\mathrm{d}\omega'}{\omega'}\tanh\frac{\omega'}{2T_{\mathrm{c}}}\,I(\omega, \omega')\lambda_{10}\Delta_1(\omega) - \varkappa_{10},
\end{aligned} \tag{14}$$

$$\begin{aligned}
&Z_{00}(\omega)\Delta_1(\omega) + \frac{\lambda_{01}(\omega)\Delta_0(\omega)}{2} \\
&\quad = \int_0^{\infty} \frac{\mathrm{d}\omega'}{\omega'}\tanh\frac{\omega'}{2T_{\mathrm{c}}}\,I(\omega, \omega')\lambda_{01}\Delta_0(\omega) - \varkappa_{01} \\
&\quad + \int_0^{\infty} \frac{\mathrm{d}\omega'}{\omega'}\tanh\frac{\omega'}{2T_{\mathrm{c}}}\,I(\omega, \omega')\,\frac{\lambda_{11}}{2}\,\Delta_1(\omega) - \varkappa_{11},
\end{aligned} \tag{15}$$

where we set

$$\varkappa_{ij} = \mu_{ij}\int_0^{E_{\mathrm{F}}} \frac{\mathrm{d}\omega'}{\omega'}\tanh\frac{\omega'}{2T_{\mathrm{c}}}\,\Delta_j(\omega). \tag{16}$$

Consequently, calculations of the critical temperature lead to solving the system of singular integral equations. Analytically solving the Eliashberg equations is impossible in general. As shown in [28, 39, 40], in the weak electron–phonon coupling approach $\lambda < 0.3$, the Eliashberg equations are transformed into the BCS equations. The strong electron–phonon coupling ($\lambda > 1$) generally requires computer simulation [28] or the McMillan approximation [41]. For intermediate values of the electron–phonon interaction $0.3 < \lambda_{ij} < 1$, the system of integral equations is solved by an iteration procedure [39, 40]. However, due to the logarithmic singularity of the kernel $I(\omega, \omega')$ at $\omega' = 0$ and $\omega = \omega''$, the iteration procedure diverges. Here, we use the Zubarev procedure of singularity removal [42]. Then system of equations (14), (15) can be rewritten as

$$\begin{aligned}
&Z_{00}(\omega)\Delta_0(\omega) + \frac{\lambda_{10}(\omega)\Delta_0(\omega)}{2} \\
&\quad = \int_0^{\infty} \frac{\mathrm{d}\omega'}{\omega'}\tanh\frac{\omega'}{2T_{\mathrm{c}}}\left[I(\omega, \omega') - I(\omega, 0)I(0, \omega')\right]\lambda_{00}\Delta_{00}(\omega) \\
&\quad - \varkappa_{00} + I(\omega, 0)\left[\Delta_0(0) + \varkappa_{00}\right] \\
&\quad + \int_0^{\infty} \frac{\mathrm{d}\omega'}{\omega'}\tanh\frac{\omega'}{2T_{\mathrm{c}}}\,I(\omega, \omega')\lambda_{10}\Delta_1(\omega) - \varkappa_{10} \\
&\quad + I(\omega, 0)\left(\Delta_{10}(0) + \varkappa_{10}\right),
\end{aligned} \tag{17}$$

$$
\begin{aligned}
&Z_{00}(\omega)\Delta_1(\omega)+\frac{\lambda_{01}(\omega)\Delta_0(\omega)}{2}\\
&=\int_0^\infty\frac{\mathrm{d}\omega'}{\omega'}\tanh\frac{\omega'}{2T_\mathrm{c}}\big[I(\omega,\omega')-I(\omega,0)I(0,\omega')\big]\lambda_{01}\Delta_{01}(\omega)\\
&-\varkappa_{01}+I(\omega,0)\big(\Delta_1(0)+\varkappa_{01}\big)\\
&+\int_0^\infty\frac{\mathrm{d}\omega'}{\omega'}\tanh\frac{\omega'}{2T_\mathrm{c}}\,I(\omega,\omega')\,\frac{\lambda_{11}}{2}\,\Delta_1(\omega)-\varkappa_{11}\\
&+I(\omega,0)\big(\Delta_{11}(0)+\varkappa_{11}\big)\,,
\end{aligned}
\tag{18}
$$

where

$$
\Delta_{ij}(0)=I(\omega,0)+\varkappa_{ij}\big(I(\omega,0)-1\big)\,.
$$

The last system of integral equations has no singularities and as a result the iteration procedure converges. System of integral equations (17), (18) gives the critical temperature. Calculating the integrals, we obtain the system of algebraic equations

$$
\Big[Z_{00}-(\lambda_{00}-\mu_{00}^*)x\Big]\Delta_0+\left[\frac{\lambda_{10}}{2}-\left(\frac{\lambda_{10}}{2}-\frac{\mu_{10}^*}{2}\right)x\right]\Delta_1=0\,, \tag{19}
$$

$$
\Big[\lambda_{01}-(\lambda_{01}-\mu_{01}^*)x\Big]\Delta_0+\left[Z_{00}-\left(\frac{\lambda_{11}}{2}-\frac{\mu_{11}^*}{2}\right)x\right]\Delta_1=0\,, \tag{20}
$$

where

$$
x=\ln\frac{1.13\omega_\mathrm{ln}}{T_\mathrm{c}}\,, \tag{21}
$$

and ω_ln is defined as

$$
\omega_\mathrm{ln}=\exp\langle\ln\omega\rangle=\exp\left\langle\frac{\int\mathrm{d}\omega\,S(\omega)/\omega\,\ln\omega}{\int\mathrm{d}\omega\,S(\omega)/\omega}\right\rangle, \tag{22}
$$

$$
\mu_{ij}^*=\frac{\mu_{ij}}{1+\mu_{ij}\ln\left(E_\mathrm{F}/\omega_\mathrm{ln}\right)}\,. \tag{23}
$$

From the vanishing of the determinant of system of equations (19), (20), we obtain the following explicit expression for the critical temperature:

$$
T_\mathrm{c}=1.134\omega_\mathrm{ln}\exp\left(-x_\mathrm{min}\right), \tag{24}
$$

where

$$
\begin{aligned}
x_\mathrm{min}&=\frac{1}{(\lambda_{00}-\mu_{00}^*)(\lambda_{11}-\mu_{11}^*)-(\lambda_{10}-\mu_{10}^*)(\lambda_{01}-\mu_{01}^*)}\\
&\times\left\{Z_{00}(\lambda_{00}-\mu_{00}^*)+\frac{Z_{00}(\lambda_{11}-\mu_{11}^*)}{2}\right.\\
&\left.-\frac{1}{2}\big[(\lambda_{01}-\mu_{01}^*)\lambda_{10}+(\lambda_{10}-\mu_{10}^*)\lambda_{01}\big]-F^{1/2}\right\},
\end{aligned}
\tag{25}
$$

$$
\begin{aligned}
F&=\left\{Z_{00}(\lambda_{00}-\mu_{00}^*)+\frac{Z_{00}(\lambda_{11}-\mu_{11}^*)}{2}\right.\\
&\left.-\frac{1}{2}\big[(\lambda_{01}-\mu_{01}^*)\lambda_{10}+(\lambda_{10}-\mu_{10}^*)\lambda_{01}\big]\right\}^2\\
&-2\big[(\lambda_{00}-\mu_{00}^*)(\lambda_{11}-\mu_{11}^*)-(\lambda_{10}-\mu_{10}^*)(\lambda_{01}-\mu_{01}^*)\big]\\
&\times\left(Z_{00}^2-\frac{\lambda_{10}\lambda_{01}}{2}\right).
\end{aligned}
\tag{26}
$$

2.2 Nonadibaticity effects in layered systems

In the case of nonadiabatic anisotropic superconductors ($m\leqslant 1$), the generalized Eliashberg equations describing pairing in systems with a cylindrical symmetry have the form [30, 31]

$$
\begin{aligned}
Z(p_z,\omega_n)\Delta(p_z,\omega_n)&=\pi T_\mathrm{c}\int_{-\pi}^{\pi}\frac{\mathrm{d}(p_z'd)}{2\pi}\\
&\times\sum_m\frac{\lambda_\Delta(p_z,p_z',\omega_n,\omega_m,Q_\mathrm{c};\omega_0,E)}{(\omega_n-\omega_m)^2+\omega_0^2}\,\omega_0^2\,\frac{\Delta(p_z',\omega_m)}{|\omega_m|}\\
&\times\frac{2}{\pi}\arctan\frac{E}{2Z(p_z',\omega_m)|\omega_m|}\,,
\end{aligned}
\tag{27}
$$

$$
\begin{aligned}
Z(p_z,\omega_n)&=1+\frac{\pi T_\mathrm{c}}{\omega_n}\int_{-\pi}^{\pi}\frac{\mathrm{d}(p_z'd)}{2\pi}\\
&\times\sum_m\frac{\lambda_z(p_z,p_z',\omega_n,\omega_m,Q_\mathrm{c};\omega_0,E)}{(\omega_n-\omega_m)^2+\omega_0^2}\,\omega_0^2\,\frac{\omega_m}{|\omega_m|}\\
&\times\frac{2}{\pi}\arctan\frac{E}{2Z(p_z',\omega_m)|\omega_m|}\,,
\end{aligned}
\tag{28}
$$

where $Z(p_z,\omega_n)$ is a renormalization parameter, $\Delta(p_z,\omega_n)$ is the energy gap, and E is the total bandwidth, with the energy defined in the interval $-E/2<\mathcal{E}<E/2$, Q_c is the cut-off parameter for the phonon momentum transfer $Q_\mathrm{c}=q_\mathrm{c}/2k_\mathrm{F}$, and $\omega_m=(2m-1)\pi k_\mathrm{B}T_\mathrm{c}$ are the Matsubara frequencies ($m=0,\pm1,\pm2,\dots$). We use the following standard notation for the effective couplings:

$$
\begin{aligned}
\lambda_\Delta(p_z,p_z',\omega_n,\omega_m,Q_\mathrm{c};\omega_0,E)&=\lambda(p_z,p_z')\\
&\times\big[1+2\lambda(p_z,p_z')\,P_\mathrm{v}(p_z,p_z',\omega_n,\omega_m,Q_\mathrm{c};\omega_0,E)\\
&+\lambda(p_z,p_z')\,P_\mathrm{c}(p_z,p_z',\omega_n,\omega_m,Q_\mathrm{c};\omega_0,E)\big]\,,
\end{aligned}
\tag{29}
$$

$$
\begin{aligned}
\lambda_z(p_z,p_z',\omega_n,\omega_m,Q_\mathrm{c};\omega_0,E)&=\lambda(p_z,p_z')\\
&\times\big[1+\lambda(p_z,p_z')\,P_\mathrm{v}(p_z,p_z',\omega_n,\omega_m,Q_\mathrm{c};\omega_0,E)\big]\,.
\end{aligned}
\tag{30}
$$

The general expressions for the so-called vertex and cross functions P_v and P_c were given in [34–36]. The vertex and cross functions are expanded in terms of Fermi-surface harmonics [28], which form a complete, orthonormal set of functions on the Fermi surface. For our model energy spectrum [Eqn (6)], Fermi-surface harmonics can be represented by $\cos(np_zd)$. The anisotropic electron–phonon coupling parameter $\lambda(p_z,p_z')$ without the corrections in Eqns (29) and (30) is expanded as in (11) with $\lambda_{01}=\lambda_{10}$. As noted in [37, 38], the off-diagonal elements of the electron–phonon interaction in layered systems with the electron spectrum in Eqn (6) and quasi-two-dimensional phonon spectra [Eqns (7) and (8)] are proportional to t/E_F. As shown in [43, 44], layered systems are characterized by low-frequency optical phonons, which correspond to the oscillations of planes as rigid molecules with respect to one another. As noted in [45–47], low-frequency phonons play a significant role in superconductors with a weak electron–phonon coupling. In the opposite case, i.e., in the strong-coupling limit, the critical temperature T_c is determined by the high-frequency peculiarities in the phonon spectrum.With this argument in mind, we take the interaction of electrons with acoustic in-plane phonons (7), (8) into account.

For layered systems, the above condition implies that $\lambda_{11}\ll\lambda_{01}<\lambda_{00}$, which suggests that we can neglect terms of the order $\lambda_{11}/\lambda_{01}$ and $\lambda_{11}/\lambda_{00}$ in subsequent calculations. For the calculation of λ_{00} and λ_{01}, we use the expression for the

electron–phonon interaction without the vertex correction in Eqn (29). In a more general situation, we have the following expressions for the vertex-corrected interaction [for convenience, other arguments are omitted in (29) and (30)]:

$$\lambda_{\Delta}(p_z, p_z') = \lambda(p_z, p_z') \times \left[1 + 2\sum_{k_z} \lambda(k_z - p_z)\, G(k_z)\, G(p_z' - p_z + k_z)\right] + \lambda(p_z, p_z') \sum_{k_z} \lambda(k_z - p_z)\, G(k_z)\, G(k_z - p_z - p_z')\,, \quad (31)$$

$$\lambda_z(p_z, p_z') = \lambda(p_z, p_z') \times \left[1 + \sum_{k_z} \lambda(k_z - p_z)\, G(k_z)\, G(k_z - p_z + p_z')\right]. \quad (32)$$

For a small parameter $t/T_c \ll 1$, and at temperatures close to T_c, the Green's functions of electrons can be expressed as

$$G(\mathrm{i}\omega_n, p, p_z) = \frac{1}{\mathrm{i}\omega_n - \xi(p, p_z)} \approx \frac{1}{\mathrm{i}\omega_n - \xi(p)}\left[1 + \frac{t\cos(p_z d)}{\mathrm{i}\omega_n - \xi(p)}\right], \quad (33)$$

where $\xi(p, p_z) = E(p, p_z) - \mu$ and μ is the chemical potential. With Eqns (10)–(12), we obtain the final expression for the vertex-corrected electron–phonon interaction:

$$\lambda_{\Delta} = \lambda_{00} + \lambda_{00}^2(2P_v + P_c) + \lambda_{01}\left[1 + 2\lambda_{00}(2P_v + P_c)\right]\cos(p_z d) + \lambda_{10}\left[1 + \lambda_{00}(2P_v + P_c)\right]\cos(p_z' d) + \lambda_{00}\lambda_{10}(2P_v + P_c)\cos(p_z d - p_z' d)\,, \quad (34)$$

$$\lambda_z = \lambda_{00} + \lambda_{00}^2 P_v\,. \quad (35)$$

In the model of Fermi-surface harmonics, the order parameter takes form (12). As shown in [34], the critical temperature T_c can be obtained from the generalized Eliashberg equations by an analytic approach. The final expression for T_c beyond the adiabatic limit in s-wave isotropic superconductors for an arbitrary momentum transfer is given by [34–36]

$$T_c = \frac{1.13\,\omega_0}{(1+m)\mathrm{e}^{1/2}} \exp\frac{m}{2+2m} \exp\left[-\frac{1 + \lambda_z/(1+m)}{\lambda_{\Delta}}\right]. \quad (36)$$

Substituting Eqns (34), (35), and (12) in (27) and (28), and using the McMillan approximation [41], we have the system of algebraic equations

$$\left(1 + \frac{\lambda_z^{00}}{1+m} - \lambda_{\Delta}^{11} x\right)\Delta_0 + \lambda_{\Delta}^{10} x \Delta_1 = 0\,, \quad (37)$$

$$\lambda_{\Delta}^{10} x \Delta_0 + \left(1 + \frac{\lambda_z^{00}}{1+m} - \lambda_{\Delta}^{11} x\right)\Delta_1 = 0\,, \quad (38)$$

where

$$x = \ln\frac{1.13\,\omega_0}{T_c} - \ln(1+m) - \frac{1 - m/(1+m)}{2}\,, \quad (39)$$

$$\lambda_z^{00} = \lambda_{00} + \lambda_{00}^2 P_v\,, \quad (40)$$

$$\lambda_{\Delta}^{00} = \lambda_{00} + \lambda_{00}^2(2P_v + P_c)\,, \quad (41)$$

$$\lambda_{\Delta}^{01} = \lambda_{01} + 2\lambda_{00}\lambda_{01}(2P_v + P_c)\,, \quad (42)$$

$$\lambda_{\Delta}^{11} = \lambda_{00}\lambda_{11}(2P_v + P_c)\,. \quad (43)$$

From the vanishing of the determinant of system (37), (38) and the condition $t/E_F \ll 1$, we obtain the explicit formula for the critical temperature

$$\frac{T_c}{T_{c0}} = \exp\left[\kappa\left(\frac{\lambda_{01}}{\lambda_{00}}\right)^2\right], \quad (44)$$

where T_{c0} is the critical temperature without the vertex corrections and

$$\kappa = \frac{1}{2}\,\frac{1 + \lambda_{00}(1 + \lambda_{00}P_v)/(1+m)}{\lambda_{00}\left[1 + \lambda_{00}(2P_v + P_c)\right]}\,\frac{(1 + \lambda_{00}P_v)/(1+m)}{\lambda_{00}\left[1 + \lambda_{00}(2P_v + P_c)\right]}\,. \quad (45)$$

The coefficient κ embodies the effects of vertex corrections and anisotropy in determining T_c. The explicit forms of the vertex correction P_v and the cross correction P_c in the two-dimensional case are given in [48].

2.3 Effect of Coulomb repulsion in layered superconductors

To obtain the average value μ of the screened Coulomb potential $\tilde{V}(\mathbf{k}, k_z)$ over a quasi-two-dimensional Fermi surface, we use the formula [32]

$$\mu = \frac{D}{2\pi}\int_{-\pi/D}^{\pi/D} \mathrm{d}k_z\,\frac{2N_{2D}(0)}{\pi}\int_0^{2p_F^*}\frac{\mathrm{d}\mathbf{k}}{\left[(2p_F^*)^2 - k^2\right]^{1/2}}\,\tilde{V}(\mathbf{k}, k_z)\,, \quad (46)$$

where $N_{2D}(0)$ is the two-dimensional density of states on the Fermi surface and p_F^* is given by $(2p_F^*)^2 = (2p_F)^2 - 4mt[1 - \cos(p_z d)]$, $D = a + d$, where d is the thickness of the conducting layer and a is the distance between them.

To calculate μ, we use the expression for the bare Coulomb potential $V(\mathbf{k}, k_z)$ rewritten for a superlattice with different dielectric constants. Such a potential was obtained in Ref. [49] and has the form

$$V\big(n(a+d), k\big) = \frac{2\pi e}{\epsilon_1 k}\exp(-nk_0)\,\frac{(1+\gamma_1)(1-\gamma_2)}{\gamma_1 - \gamma_2}\,, \quad (47)$$

where

$$\gamma_1 = \frac{\exp(ka) - \exp k_0\left[\alpha\exp(-kd) + \beta\exp(kd)\right]}{\exp(-ka) - \exp k_0\left[\beta\exp(-kd) + \alpha\exp(kd)\right]}\,, \quad (48)$$

γ_2 can be obtained from the expression for γ_1 by changing the sign of k_0, and k_0 is given as

$$k_0 = \operatorname{arcosh}\left\{\cosh\left[k(a-d)\right] + \frac{2\alpha^2}{2\alpha - 1}\sinh(ka)\sinh(kd)\right\}. \quad (49)$$

The other dimensionless parameters are $\alpha = (1+\eta)/2$, $\beta = (1-\eta)/2$, and $\eta = \epsilon_1/\epsilon$, where ϵ and ϵ_1 are respectively the static dielectric constants of the metal and the dielectric. Using the expression for the Fourier transform [50]

$$\sum_n \exp(-nk_0)\exp\left[-\mathrm{i}nk_z(a+d)\right] = \frac{\sinh k_0}{\cosh k_0 - \cos\left[k_z(a+d)\right]}\,, \quad (50)$$

we finally obtain

$$V(k,k_z)=\frac{2\pi e}{\epsilon k}\times\frac{\alpha\sinh\left[k(a+d)\right]+\beta\sinh\left[k(a-d)\right]}{\alpha^2\cosh\left[k(a+d)\right]-\beta^2\cosh\left[k(a-d)\right]-\eta\cos\left[k_z(a+d)\right]}\,. \tag{51}$$

In the case where $a\gg d$, we obtain the expression for the Coulomb potential for a layered system filled by a medium with a static dielectric constant ϵ_1:

$$V(k,k_z)=\frac{2\pi e}{\epsilon_1 k}\,\frac{\sinh(ka)}{\cosh(ka)-\cos(k_z a)}\,. \tag{52}$$

For $a\ll d$, substitutions $\epsilon_1\to\epsilon$ and $a\to d$ must be made in Eqn (52).

The screened Coulomb potential $\tilde{V}(\mathbf{q},q_z;\omega)$ can be expressed in terms of the electron polarization operator $\Pi(\mathbf{q},q_z;\omega)$ as

$$\tilde{V}(\mathbf{q},q_z;\omega)=\frac{V(\mathbf{q},q_z)}{1+V(\mathbf{q},q_z)\,\Pi(\mathbf{q},q_z;\omega)}\,. \tag{53}$$

The polarization operator $\Pi(\mathbf{q},q_z;\omega)$ is given by [51]

$$\Pi(\mathbf{q},q_z;\omega)=2\sum_{\mathbf{p},p_z}\frac{n\big(\xi(\mathbf{p}+q,p_z+q_z)\big)-n\big(\xi(\mathbf{p},p_z)\big)}{\xi(\mathbf{p},p_z)-\xi(\mathbf{p}+\mathbf{q},p_z+q_z)+\mathrm{i}\omega}\,, \tag{54}$$

where $n(\ldots)$ is the Fermi distribution. In the case of the energy spectrum in Eqn (6) at zero frequency, we obtain

$$\frac{\Pi(q,q_z,0)}{\Pi(0)}=1-\frac{1}{q^2}\int_{-\pi/(a+d)}^{\pi/(a+d)}\frac{\mathrm{d}p_z}{2\pi}\times\left[A^2-(2qq^*)^2\right]^{1/2}v\left[A^2-(2qq^*)^2\right]\operatorname{sgn}A\,, \tag{55}$$

where

$$\Pi(0)=\frac{m}{\pi\hbar^2}\,,\quad A=q^2+4mt\sin\frac{q_z(a+d)}{2}\sin\left[p_z(a+d)\right],$$
$$q^*=\left\{q_{\mathrm{F}}^2-2mt\left[1-\cos\left(p_z-\frac{q_z}{2}\right)(a+d)\right]\right\}^{1/2}.$$

For the functions $v(x)$ and $\operatorname{sgn}(x)$, $v(x)=1$ for $x>0$, $v(x)=0$ for $x<0$, $\operatorname{sgn}(x)=1$ for $x>0$, and $\operatorname{sgn}(x)=-1$ for $x<0$. From the last expression, the polarization operator $\Pi(\mathbf{q},q_z;0)$ remains constant over a wide range of $\mathbf{q}$, and there are corrections in the vicinity of $2p_{\mathrm{F}}$.

2.4 Plasmon spectrum of layered superconductors

Plasmon modes can be found as poles of the Dyson equation for the Coulomb potential, which has the form of expression (53). To calculate the plasmon spectrum, we use the expression for the bare Coulomb interaction $V(\mathbf{q},q_z)$ [49] of charged particles in a periodic layered system consisting of alternating layers with different values of the dielectric constant in the long-wavelength approximation. It is clear that as the thickness of the conducting layer increases, the Coulomb repulsion decreases. Using Eqns (53)–(55), we can obtain the final expression for the plasmon spectrum in layered superconductors as

$$\omega^2(q,q_z)=\left(v_{\mathrm{F}}^2q^2+8t^2\sin^2\frac{q_zD}{2}\right)\Pi(0)V(q,q_z)\,, \tag{56}$$

where v_{F} is the velocity of electrons on the Fermi surface. For $t=0$, $q_z\to 0$, and $qD\gg 1$, we obtain the spectrum of two-dimensional plasmons in the long-wavelength approximation:

$$\omega(q)=v_{\mathrm{F}}\left(\frac{2q}{a_{\mathrm{B}}}\right)^{1/2}, \tag{57}$$

where $a_{\mathrm{B}}=1/(me^2)$ is the Bohr radius for a free electron. For $qD\ll 1$ and $q_zD\ll 1$, the plasma frequency depends on the direction of the wave vector:

$$\omega(q,q_z)=\left(\frac{2}{a_{\mathrm{B}}D}\right)^{1/2}\left[v_{\mathrm{F}}^2+(t^2D^2-v_{\mathrm{F}}^2)\cos^2\theta\right]^{1/2}, \tag{58}$$

where θ is the angle between the wave vector and the vector normal to the layer. As follows from Eqn (58), the spectrum of plasmons is strongly anisotropic. The frequency of plasma oscillations with the wave vector perpendicular to the layer is $v_{\mathrm{F}}/(tD)\gg 1$ times smaller than the plasma frequency in the layer [52].

2.5 Specific heat jump of layered superconductors

In the case of a weak electron–phonon coupling, Eliashberg equations (3) and (4) are transformed into the BCS equation [40]

$$Z(\omega)=1\,, \tag{59}$$

$$\Delta(p_z)=\int_{-\pi}^{\pi}\frac{\mathrm{d}p_z'}{2\pi/d}\int_0^{\infty}\frac{\mathrm{d}^2p}{(2\pi)^2}\times\frac{\tanh\left\{\left[\xi^2(p-p',p_z-p_z')+\Delta^2(p-p',p_z-p_z')\right]^{1/2}/(2T)\right\}}{\left[\xi^2(p-p',p_z-p_z')+\Delta^2(p-p',p_z-p_z')\right]^{1/2}}\times V_{p_z,p_z'}\,\Delta(p_z')\,, \tag{60}$$

where ξ is energy spectrum (6) referenced to the chemical potential μ, and the pairing potential $V(p_z,p_z')$ can be expressed similarly to (11). In Eqn (60), we neglect the Coulomb potential. The solution of the linearized BCS equation at T_{c} is given by (12). In the vicinity of the critical temperature T_{c}, the value of Δ_i can be expanded into a series in the small parameter $t^{1/2}=(1-T/T_{\mathrm{c}})^{1/2}$, $\Delta_i=c_it^{1/2}+c_i't^{3/2}+\ldots$. It then follows from Eqn (60) that

$$(x\lambda_{00}-1)c_0+\frac{\lambda_{01}xc_1}{2}=0\,, \tag{61}$$

$$\left(\frac{x\lambda_{11}}{2}-1\right)c_1+\lambda_{01}xc_0=0\,, \tag{62}$$

where $\lambda_{ij}=N^{2\mathrm{D}}(0)V_{ij}$, and $N^{2\mathrm{D}}(0)$ represents the two-dimensional density of states. These equations determine the critical temperature T_{c} and the ratio of order parameters c_0/c_1. In what follows, we introduce the ratio of order parameters at a temperature close to T_{c}:

$$\chi=\left.\frac{\Delta_0}{\Delta_1}\right|_{T=T_{\mathrm{c}}}=\frac{c_0}{c_1}=\frac{(\lambda_{01}/2)x}{1-\lambda_{00}x}=\frac{1-(\lambda_{11}/2)x}{\lambda_{01}x}\,, \tag{63}$$

where $x=\ln(\omega_0/T_{\mathrm{c}})$ and ω_0 is the Debye frequency. The behavior of the order parameters Δ_0 and Δ_1 at temperatures close to the critical temperature can be calculated from Eqn (60) and then rewritten using the Matsubara technique. Expanding the right-hand side in powers of

Δ_0^2/T_c^2, we have [51]

$$\Delta(p_z) = T\sum_n \int_{-\pi}^{\pi} \frac{dp_z'}{2\pi/d} \int_{-\omega_0}^{\omega_0} d\xi\, \lambda(p_z, p_z')\, \Delta(p_z') \times \left[\frac{1}{\omega_n^2 + \xi^2} - \frac{\Delta^2(p_z')}{(\omega_n^2 + \xi^2)^2}\right], \quad (64)$$

where $\omega_n = (2n-1)\pi kT$ (with $n = 0, \pm1, \pm2, \ldots$) are the Matsubara frequencies. Substituting the expression for $\Delta(p_z)$ in the last equation and then calculating the integrals and equating the coefficients at the same harmonics, we have

$$\Delta_0 = \ln\frac{\omega_0}{T}\left(\lambda_{00}\Delta_0 + \frac{\lambda_{01}}{2}\Delta_1\right) - \frac{7\zeta(3)}{8\pi^2 T_c^2}\left[\lambda_{00}\left(\Delta_0^3 + \frac{3}{2}\Delta_0\Delta_1^2\right) + \frac{\lambda_{10}}{2}\left(3\Delta_0^2\Delta_1 + \frac{4}{3}\Delta_1^3\right)\right], \quad (65)$$

$$\Delta_1 = \ln\frac{\omega_0}{T}\left(\lambda_{01}\Delta_0 + \frac{\lambda_{11}}{2}\Delta_1\right) - \frac{7\zeta(3)}{8\pi^2 T_c^2}\left[\lambda_{01}\left(\Delta_0^3 + \frac{3}{2}\Delta_0\Delta_1^2\right) + \frac{\lambda_{11}}{2}\left(3\Delta_0^2\Delta_1 + \frac{4}{3}\Delta_1^3\right)\right], \quad (66)$$

where $\zeta(x)$ is the Riemann zeta function. Using that $\ln(\omega_0/T) = x + \ln(1+t) \approx x + t$, after a series of transformations, we obtain following expression for c_0:

$$c_0^2 = \frac{8\pi^2 T_c^2}{7\zeta(3)} \frac{8\chi^4 + 4\chi^2}{8\chi^4 + 24\chi^2 + 3}. \quad (67)$$

To calculate the specific heat jump of layered superconductors at the critical temperature, we use the expression [53]

$$C_S - C_N = \beta_c^3 \sum_{p,p_z} \frac{\partial\Delta^2(p_z)}{\partial\beta}\bigg|_{\beta=\beta_c} \frac{\exp(\beta\varepsilon(p,p_z))}{(1+\exp(\beta\varepsilon(p,p_z)))^2}, \quad (68)$$

where $\beta = 1/T$. Passing from summation to the integration over momenta with quasi-two-dimensional spectrum (6) for $t/\mu \ll 1$, we arrive at

$$C_S - C_N = N^{2D}(0)\frac{8\pi^2 T_c^2}{7\zeta(3)} \frac{8\chi^4 + 8\chi^2 + 2}{8\chi^4 + 24\chi^2 + 3}. \quad (69)$$

Using the expression for the specific heat in the normal case [54], we finally obtain the normalized specific heat jump in layered superconductors as [55]

$$\frac{C_S - C_N}{C_N} = 1.43 \frac{8\chi^4 + 8\chi^2 + 2}{8\chi^4 + 24\chi^2 + 3}. \quad (70)$$

2.6 Fluctuation effects on the critical temperature in layered superconductors

To study the effects of the order parameter phase fluctuations on the critical temperature T_c, we start from the Lawrence–Doniach free energy functional $F[\phi]$ for quasi-two-dimensional superconductors [56]:

$$F[\phi] = N_S^{2D}\sum_j \int d^2r \left\{\frac{\hbar^2}{8m}\left(\frac{\partial\phi_j}{\partial r}\right)^2 + \sum_{g=\pm1} W_\perp\left[1 - \cos\left(\phi_j(r) - \phi_{j+g}(r)\right)\right]\right\}, \quad (71)$$

where $\phi_j(r)$ is the phase of the order parameter $\Delta_j = |\Delta_j|\exp(i\phi_j(r))$ in the plane j with coordinates $r = (x, y)$, $W_\perp = t^2/\mu$ is the Josephson energy, and $N_S^{2D}(T)$ is the surface concentration of superconducting electrons defined as

$$N_S^{2D}(T) = N_S^{2D}(0)\left(1 - \frac{T}{T_{c0}^{2D}}\right) = \frac{p_F^2}{2\hbar^2}\left(1 - \frac{T}{T_{c0}^{2D}}\right). \quad (72)$$

In (71), the contribution of the modulus of the order parameter is neglected. The mean value of the order parameter is defined by

$$\langle\cos\phi_j\rangle = \frac{\int D\phi \cos\phi_j \exp\left(-F_{st}[\phi]/(kT)\right)}{\int D\phi \exp\left(-F_{st}[\phi]/(kT)\right)}. \quad (73)$$

Exact calculation of integral (73) with free energy functional (71) is not possible. At $T = T_c$, Eqn (73) with free energy functional (71) has a nonzero solution, which may define the transition temperature T_c. To calculate integral (73), we use the mean field approximation by replacing free energy functional (71) with

$$\hat{F}[\phi] = N_S^{2D}\sum_j \int d^2r \left[\frac{\hbar^2}{8m}\left(\frac{\partial\phi_j}{\partial r}\right)^2 + W_\perp\langle\cos\phi\rangle\cos\phi\right] = F_0 - N_S^{2D}W_\perp\langle\cos\phi\rangle\int d^2r\, \cos\phi(r), \quad (74)$$

where $F_0[\phi]$ is the free energy functional of a two-dimensional superconductor and $W_\perp = \sum_g W_\perp(g)$. In the vicinity of T_c, the order parameter tends to zero. Therefore, the second part of the free energy potential $\hat{F}[\phi]$ may be chosen as a small parameter. Substituting (74) instead of $F_{st}[\phi]$ in (73) and performing transformations, we obtain the following equation for T_c:

$$1 = \frac{N_S^{2D}(T)W_\perp}{kT_c}\int d^2r \left\langle\cos\phi(0)\cos\phi(r)\right\rangle_0, \quad (75)$$

where $\langle\ldots\rangle_0$ indicates averaging with the free energy functional $F_0[\phi]$ for a single superconducting layer. The correlator $\langle\cos\phi(0)\cos\phi(r)\rangle_0$ has been calculated in [57] and has the form

$$\left\langle\cos\phi(0)\cos\phi(r)\right\rangle_0 = \begin{cases} \left(\dfrac{\xi_{2D}}{r}\right)^{(1/\pi)\left(kT/\left[E_F(1-T/T_{c0}^{2D})\right]\right)} & \text{if } r > \xi_{2D}, \\ \exp\left[-\dfrac{1}{\pi}\dfrac{kT}{E_F(1-T/T_{c0}^{2D})}\left(\dfrac{r}{\xi_{2D}}\right)^2\right] & \text{if } r < \xi_{2D}, \end{cases} \quad (76)$$

where $\xi_{2D} = \hbar v_F/(\pi\Delta(0))$ is the correlation length inside the superconducting plane. Equation (75) may be solved for T_c with correlator (76) if the following condition is satisfied:

$$\frac{1}{2\pi}\frac{kT_c}{E_F(1 - T_c/T_{c0}^{2D})} < 1. \quad (77)$$

This means that

$$T_c^* < T < T_{c0}^{2D}, \quad (78)$$

where T_c^*, defined as

$$\frac{1}{kT_c^*} = \frac{1}{kT_{c0}^{2D}} + \frac{1}{2\pi E_F}\,, \tag{79}$$

is the temperature above which the interlayer phase coherence is destroyed, and T_{c0}^{2D} is the critical temperature of an individual layer. Substituting (76) in (75) under condition (77), we obtain the following expression for the critical temperature T_c:

$$\frac{1}{T_c} = \frac{1}{T_{c0}^{2D}} - \frac{1}{2\pi\xi_{2D}^2 N^{2D}(0) W_\perp} \times \left[1 - \left(1 + \frac{2\xi_{2D}^2 N^{2D}(0) W_\perp}{E_F}\right)^{1/2}\right]. \tag{80}$$

For small values of the tunneling integral $W_\perp < \hbar^2/(2m\xi_{2D}^2)$, the last equation becomes

$$T_c = T_c^*\left[1 - \frac{T_c^*}{2\pi}\frac{2m\xi_{2D}^2}{\hbar^2}\left(\frac{t}{E_F}\right)^2\right]^{-1}. \tag{81}$$

In the opposite case $W_\perp > \hbar^2/(2m\xi_{2D}^2)$, the critical temperature is given by [58]

$$T_c = \frac{T_{c0}^{2D}}{1 + T_c^{2D}/(\pi k_F \xi_{2D} t)}\,. \tag{82}$$

3. Results and discussions

3.1 T_c of layered superconductors: the case of MgB_2

Using full anisotropic Eliashberg equations (24)–(26), we have calculated the critical temperature of MgB_2 [59] . The matrix elements taken from [29] are $\lambda_{00} = 1.017$, $\lambda_{11} = 0.448$, $\lambda_{01} = 0.212$, and $\lambda_{10} = 0.115$. For the Coulomb pseudopotentials μ_{ij}^*, the Golubov values were used: $\mu_{00}^* = 0.21$, $\mu_{11}^* = 0.172$, $\mu_{01}^* = 0.095$, and $\mu_{10}^* = 0.069$. The logarithmically averaged value of the phonon frequency ω_{ln} was taken from [60]: $\omega_{ln} = 480$ K. For these parameters, the result is $T_c = 42.92$ K. Very recently, Mitrovich [61] used the following Coulomb pseudopotentials for calculations: $\mu_{00}^* = \mu_{11}^* = 0.139$, $\mu_{01}^* = \mu_{10}^* = 0.027$. The electron–phonon interaction parameters are the same as in [29]. With this set of parameters and for the logarithmically averaged value of the phonon frequency $\omega_{ln} = 767-806$ K [62], we find from the above expressions that the critical temperature is in the range 45.83–50.5 K. It is clear that our results overestimate the critical temperature of magnesium diboride. In our opinion, this is because we neglected the effects of nonadiabaticity in MgB_2. The high phonon frequency of the boron atoms ($\omega_{ph} = 0.1$ eV) indicates that MgB_2 could be in the nonadiabatic regime of the electron–phonon interaction (with the Fermi level $E_F = 0.5$ eV) [63]. In our opinion, inclusion of nonadiabatic effects in this analysis would improve our results. The expression for the critical temperature of layered nonadiabatic superconductors was obtained in [30, 31]. However, the obtained results pertain to the case $\lambda_{11} \ll \lambda_{01} < \lambda_{00}$. Our case differs from this and is the subject of other investigations.

The Eliashberg equations for isotropic two-band and anisotropic superconductors have been given by numerous authors studying MgB_2 [26, 29, 61]. In all cases, numerical simulation of the system of integral equations was performed. In contrast to those works, we presented an analytic approach and a formula for the calculation of the critical temperature T_c for the intermediate electron–phonon coupling. In the calculations, first-principle data was used for the electron–phonon interaction parameter and the Coulomb repulsion. Another interesting issue is the study of the pressure dependence of the critical temperature T_c in MgB_2 and other parameters using the Eliashberg theory [64–66].

3.2 Effects of nonadiabaticity

Our main result for the effects of anisotropy on the critical temperature in layered nonadiabatic superconductors is given by Eqns (44) and (45). In Fig. 1, to assess these effects more quantitatively, we show T_c/T_{c0} as a function of $\lambda_{01}/\lambda_{00}$ for different values of Q_c (where Q_c is the cut-off parameter of the phonon momentum transfer). The explicit expressions for λ_{00} and λ_{01} with the energy spectrum in Eqn (6) were presented in [37]. These expressions involve microscopic parameters that may be obtained from the experimental data (for example, $u_\parallel$, u_z, u_T, and E_F). But our final expression for the critical temperature T_c in Eqn (44) contains only the ratio of the parameters $\lambda_{01}/\lambda_{00}$. In the case of two-dimensional superconductors, we take $\lambda_{00} = 0.5$.

In Fig. 1, the dashed curve shows the behavior of T_c without the vertex corrections. The solid curves correspond to different Q_c values in the range 0.1–0.9, from top down. We observe that the nonadiabatic corrections become more prominent for small values of Q_c. We note that κ increases as Q_c decreases. For values $Q_c = 0.9$, the coefficient κ becomes lower than in the adiabatic case. Therefore, the vertex corrections have a similar behavior in the anisotropic and isotropic superconductors when Q_c is small. The critical temperature in the nonadiabatic case is enhanced compared to the solution without the vertex and cross corrections.

The dependence of κ on the nonadiabaticity parameter m is displayed in Fig. 2 for two different values: $Q_c = 0.1$ and $Q_c = 0.9$. As can be seen in the figure, κ decreases with an increase in m in both cases. Corrections become more significant at small m and are reduced as m increases. The behavior of κ for other values of Q_c is similar to that shown in Fig. 2. Our results seem interesting and relevant in connection with cuprate compounds such as layered nonadiabatic superconductors.

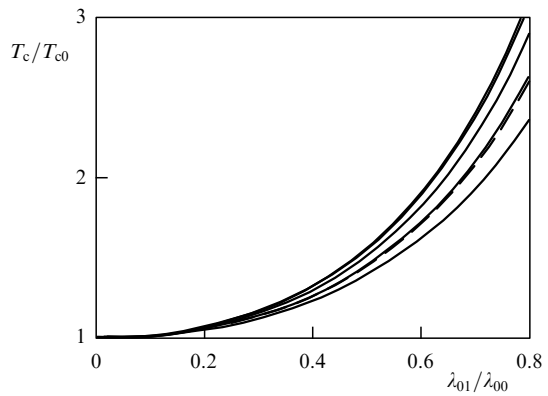

Figure 1. Critical temperature versus $\lambda_{01}/\lambda_{00}$. The dashed curve denotes the behavior of T_c without the vertex corrections. Solid curves correspond to different Q_c values in the range 0.1–0.9, from top down as Q_c increases.

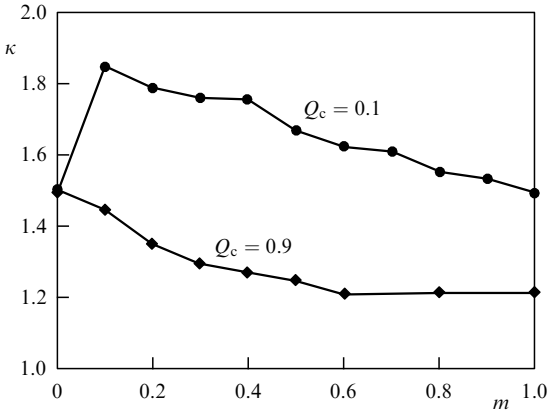

Figure 2. Dependence of κ on the nonadiabacity parameter m.

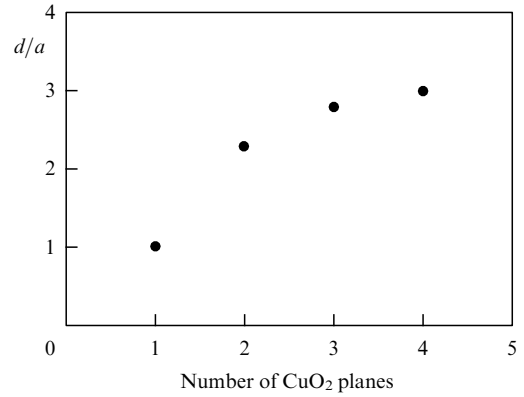

Figure 3. The ratio d/a as a function of the number n of CuO_2.

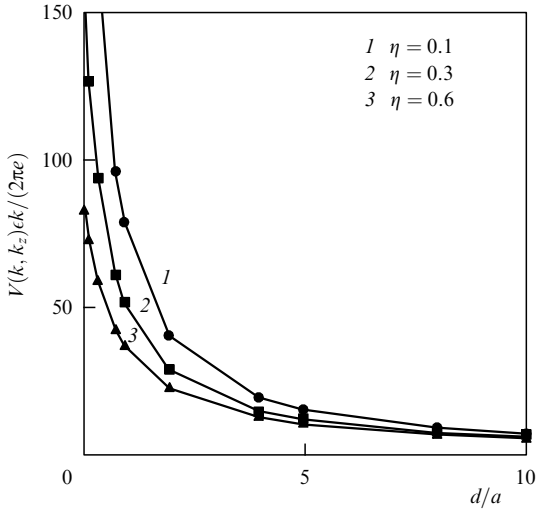

Figure 4. Coulomb repulsion as a function of d/a.

Another popular layered superconductor is Sr_2RuO_4, which has a rather low critical temperature $T_c \approx 1$ K [67]. The layered structure of the system leads to a nearly cylindrical Fermi surface that is open along the c-axis. However, there are various indications that strong correlation effects and nonadiabaticity effects are absent in Sr_2RuO_4 compounds. Therefore, in isotropic single-band s-wave nonadiabatic superconductors, vertex corrections are strongly dependent on the momentum transfer, and small values of Q_c lead to an enhancement of the critical temperature T_c [34–36].

3.3 Coulomb effects

For the Coulomb potential μ [see (46)], we can obtain analytic expressions in the different asymptotic cases. For $a > d$, the value of the Coulomb potential μ averaged over the Fermi surface is

$$\mu(a,t) = \frac{2\alpha_0}{\pi}\left(\frac{1}{\left[2p_F a\alpha_0(2\epsilon_1 + 2p_F a\alpha_0)\right]^{1/2}} + \frac{1}{\epsilon_1}\ln\frac{\alpha_0+\epsilon_1}{\alpha_0+\epsilon_1/2p_F a} + \frac{1}{\epsilon_1+\alpha_0} + \frac{4\alpha_0}{\pi\epsilon_1}\frac{(t/E_F)^{1/2}}{\epsilon_1+\alpha_0}\right), \quad (83)$$

where $\alpha_0 = e^2/(\hbar v_F)$ is the ratio of the average Coulomb potential to the kinetic energy of an electron on the Fermi surface; usually, $\alpha_0 \ll 1$. In the opposite asymptotic case $a < d$, the replacements $\epsilon_1 \to \epsilon$ and $a \to d$ must be used. Equation (83) shows that μ decreases as the thickness d of the superconducting layers increases. Such a result seems attractive for explaining the empirical Chu rule (see Ref. [11] and the references therein). According to this rule, the critical temperature of HTSCs can be calculated as

$$T_c(n) \approx 40\,n\ [\mathrm{K}]\,,$$

where n is the number of CuO_2 planes. But the dependence $T_c(n)$ saturates for $n > 5$. In our model, the thickness of the conducting layer increases as the number of CuO_2 planes increases. Our results are in good agreement with those obtained from Leggett's calculations [68, 69]. As shown in Ref. [68], the difference between the transition temperature T_c for a homologous series of n layers and the single-layer value is given by $\Delta T_c = \mathrm{const}\,(1 - 1/n)$. This is because the Coulomb energy in an n-layer structure is proportional to the number of acoustic modes ($n - 1$ acoustic modes for n layers). Consequently, the saved energy per layer can be calculated as $(n-1)/n = (1 - 1/n)$ [68]. It is useful to note that Leggett's calculations are completely independent of any 'model' or of the fundamental superconductivity mechanism in cuprates. Our approximation is related to straightforward calculations in the framework of the McMillan approach and takes the 'hard' phonon spectrum of an HTSC into account. In both calculations, T_c saturates as the number of CuO_2 planes (or the ratio d/a of the conducting layer thickness to the thickness of the dielectric) increases.

The values of a and d for different homologous cuprate series are presented in [70]. Using these data, we plot the ratio d/a as a function of the number n of CuO_2 planes (Fig. 3). The ratio d/a for HTSCs increases as n increases, which corresponds to the region in Fig. 4 where the Coulomb repulsion changes crucially, and this means that a considerable change in the critical temperature of layered SCs is induced by changing the number of CuO_2 planes. The value $d/a = 2.3$ for $n = 2$ in Fig. 3 corresponds to the $Bi_2Sr_2CaCuO_8$ compound. For another two-layer superconductor YBaCuO, the ratio $d/a = 1.73$ [70]. As shown in Refs [9, 10], the lattice static dielectric constant varies in the range 6–10 for all cuprates, and we have a value about 4 for YBaCuO [70].

To estimate $\eta = \epsilon_1/\epsilon$, we use a value of ϵ in the range 4–10, while ϵ_1 can be taken to be about 1. Consequently, η

ranges in 0.1–0.25. As Fig. 3 shows, despite the different values of d/a and η for YBaCuO and $Bi_2Sr_2CaCuO_8$ [70], the Coulomb repulsion is the same for both compounds, and therefore the critical temperatures of these compounds are nearly the same.

As a concluding remark, it is interesting to note the newly discovered superconductor magnesium diboride [13]. This material also has a layered structure with boron atoms forming layers of two-dimensional honeycomb lattices (single layer). Our results can also be applied to MgB_2 in the limit as d/a tends to zero.

It is interesting to discuss the conditions under which several atomic layers can be approximated by a continuum dielectric medium. It is well known that at the contact region of different layers in a superlattice, the crystal structure is deformed, and therefore the dielectric constant in this region is different from that in bulk material. Therefore, for our purpose of finding the dependence of the plasmon frequency on the thicknesses of the conducting and dielectric layers, the dielectric constants ϵ and ϵ_1 presented here can be considered effective dielectric constants of the layers. In our opinion, introducing a more realistic function for the change in the dielectric constant (instead of the step function used in [49]) would change our results inconsiderably. Similar questions were discussed in [71, 72] many years ago in relation to exitonic superconductivity in 'sandwich' structures.

3.4 Plasmon spectrum

The plasmon frequency for a superlattice is given by (56). For long wavelengths $(q, q_z \to 0)$, we have an optical plasmon mode (bulk plasmon):

$$\omega^2(0,0) = \frac{8E_F e^2}{\epsilon} \frac{a + \eta d}{\alpha^2(a+d)^2 - \beta^2(a-d)^2} \,. \tag{84}$$

In the other limit $q_z = \pi/D$, we obtain an acoustic plasmon mode in the lower branch. For $q_z = \pi/D$, $D = a + d$, $qD \ll 1$, and $t/E_F \ll 1$, we obtain

$$\omega(q) = \omega(0,0) \frac{\alpha^2(a+d)^2 - \beta^2(a-d)^2}{2(a+\eta d)\eta} q \,. \tag{85}$$

The plasmon spectrum of a layered superconductor has a rather complicated structure. The plasmon modes for $0 < q_z < \pi/D$ form a band, as shown in Fig. 5. The size of the band is determined by the parameter η and the ratio a/d. It is also important to note that in the limit $q_z D \to \pi$, the slope of acoustic plasmons $\mathrm{d}\omega/\mathrm{d}q$ $(q_z = \pi/D)$ is greater than in the case $q_z D = 0$.

In Fig. 6, we plot the dependence of the normalized slope of acoustic plasmon modes $\mathrm{d}\omega/\mathrm{d}q$ $(q_z = \pi/D)$ versus the ratio d/a. It is clear that by increasing the thickness of the conducting layer, the slope $\mathrm{d}\omega/\mathrm{d}q$ $(q_z = \pi/D)$ is increased. Such a conclusion is in good agreement with the numerical calculations in [73], where periodic stacks of planes were considered.

We can see that increasing the thickness of the metallic layer leads to a decrease in the plasmon frequency $\omega(0,0)$. These results can be useful for explaining the experimental data for YBaCuO $[\omega(0,0) = 2.3\ \mathrm{eV}]$ [74] and $Bi_2Sr_2CaCu_2O_8$ $[\omega(0,0) = 1\ \mathrm{eV}]$ [75, 76]. It is well known that there are two CuO_2 planes in YBaCuO and three CuO_2 planes in $Bi_2Sr_2CaCu_2O_8$ and therefore the plasmon frequency decreases. In our model, the thickness of the conducting layer increases as the number of CuO_2 planes increases. The ratio d/a for an HTSC corresponds to the region in Fig. 4 where the Coulomb repulsion changes crucially.

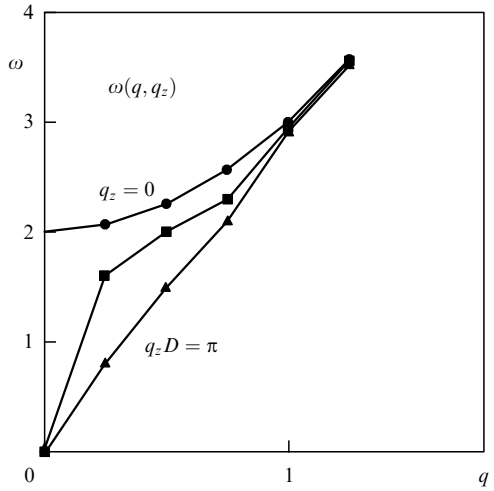

Figure 5. The plasmon modes of layered superconductors for $0 < q_z < \pi/D$; $D = a + d$ is the superlattice period.

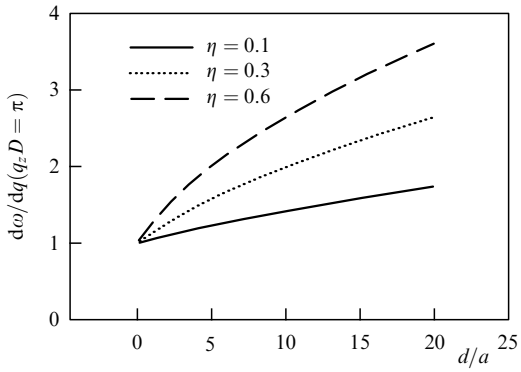

Figure 6 The dependence of the normalized slope of acoustic plasmon modes $\mathrm{d}\omega/\mathrm{d}q$ $(q_z = \pi/D)$ versus the ratio d/a.

Another interesting question is related to the influence of low-energy plasmon modes on superconductivity in layered systems. The consequences of the existence of plasmons for superconductivity were discussed by [77]. As shown in this work, low-energy plasmons can contribute constructively to superconductivity. The simplest form [Eqn (56)] of the Coulomb interaction in layered systems with zero-thickness conducting planes was considered in [77] (see also [78, 79]). The conducting sheets are stacked along the c-axis and separated by spaces with the dielectric constant ϵ_M. The electrons move within the superconducting sheets $(t = 0)$. The purpose of [77] was to investigate the increasing influence of the phonon–plasmon interaction on the electron pairing mechanism in the framework the Eliashberg theory. The plasmon contribution to superconductivity is shown to be dominant in the newly discovered layered superconductor, metal-intercalated halide nitrides [77].

Earlier, plasmon modes in layered superconductors with zero-thickness conducting planes were studied in [80] using kinetic equations for the Green's functions. It was shown that in the vicinity of T_c, plasma oscillations transformed into the Carlson–Goldman mode observed in [81]. Unlike in other studies, the influence of the order parameter on the plasmon

spectrum was also discussed. In Ref. [73], it was shown that plasmon modes that are expected in cuprate superconductors should be characteristic of a superlattice based on several metallic sheets. Numerical results were given for the superlattice plasmon dispersion relations for two and three sheets per unit cell. The electron gas in metallic sheets was considered two-dimensional. It was shown that if the spacing of the sheets is small compared to the superlattice period, then the low-frequency plasmon branches are essentially identical to those of an isolated bilayer or trilayer.

In contrast to the approaches in [73, 78, 80], we have developed a simple model with the thickness d of the conducting sheets taken into account. The value of d and the dielectric layer thickness a for different homologous cuprate series are presented in [70]. The ratio d/a for HTSCs increases as the number of CuO_2 planes per unit cell increases, which corresponds to the region in Fig. 4 where the Coulomb repulsion changes crucially and means a considerable change in the plasmon frequency of layered SCs induced by changing the number of CuO_2 planes. As noted above, the value $d/a = 2.3$ corresponds to the $Bi_2Sr_2CaCuO_8$ compound, and $d/a = 1.73$ corresponds to another cuprate, superconductor YBaCuO.

Recent studies on the growth of single crystals [18, 19] show an anisotropy of physical properties in MgB_2. Our results can also be applied to MgB_2 in the limit as d/a tends to zero. Calculations of the plasma frequency in MgB_2 using de Haas–van Alphen data were made in [82]. Another peculiarity of plasmon modes in MgB_2 is related to the two-band nature of superconductivity in this compound. In this case, the appearance of low-energy plasmon branches, so-called 'demons' [83], is the result of two overlapping bands.

3.5 Specific heat jump

It follows from (70) that $A(\chi)$ is less than unity and therefore the normalized specific heat jump in layered superconductors is smaller than in the isotropic case. This result is in qualitative agreement with paper [84], where it was shown that $A(\chi) < 1$ in the general case of anisotropic superconductors. However, the explicit expression for the specific heat jump function was not obtained there. The detailed behavior of the function $A(\chi)$ is determined by the anisotropy of the order parameter. In the case of layered superconductors with pairing in neighboring planes, the order parameter is $\Delta(p_z) = \Delta_0 + \Delta_1 \cos(p_z d)$ and it is convenient to introduce the anisotropy parameter

$$a = \frac{\Delta_{\max}}{\Delta_{\min}} = \frac{\Delta_0 + \Delta_1}{\Delta_0 - \Delta_1} = \frac{\chi + 1}{\chi - 1} \,. \tag{86}$$

The behavior of the specific heat jump as a function of the anisotropy parameter is shown in Fig. 7. The presented result can be used for the calculation of the anisotropy parameter in MgB_2. The experimental value of the specific heat jump in MgB_2 is $(C_S - C_N)/C_N = 1.18$ [60]. Using (86), we find that $a_1 = 0.5\,(\chi = -3)$ and $a_1 = 2\,(\chi = 3)$. The physical solution corresponds to the case of the positive ratio of order parameters $\chi = 3$. Similar results were obtained by computer simulation in the strong electron–phonon coupling limit in the framework of the Eliashberg theory [85] for a cylindrical Fermi surface with energy spectrum (6). The calculations show that the specific heat jump decreases with an increase in the ratio $\lambda_{01}/\lambda_{00}$ [see Eqns (63) and (69)]. We also note that the anisotropy parameter $\chi = 3$ obtained from our analytic calculations is close to the result of computer calculations performed in [29] in the framework of the isotropic two-band microscopic Eliashberg theory ($\Delta_\sigma/\Delta_\pi = 2.63$).

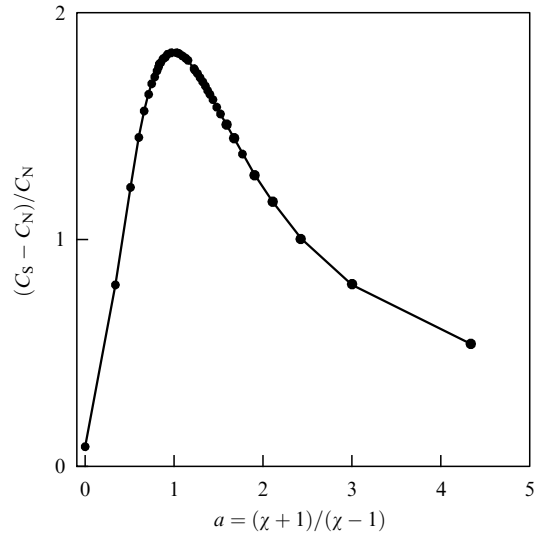

Figure 7. The behavior of the specific heat jump as a function of the anisotropy parameter a.

3.6 Order parameter fluctuations

As follows from Eqns (80)–(82), the critical temperature T_c increases with an increase in the tunneling integral t, and approaches T_c^{2D} in the interval $T_c^* < T_c < T_c^{2S}$. In the absence of Josephson coupling between planes, fluctuations of the order parameter phase would destroy the long-range order [57]. Nevertheless, the existence of topological defects in two-dimensional superconductors, such as 'vortices' and 'antivortices' of a phase field, should result in a Berezinski–Kosretlitz–Thouless phase transition at $T < T_{KT}$ [86, 87]. The same defects give rise to a quasi-long-range order for $T_{KT} < T_c < T_c^{2D}$, where T_c^{2D} is the critical temperature formally evaluated by the mean field theory for a single superconducting plane.

4. Conclusions

We have summarized a number of recent investigations of layered superconductors using the microscopic Eliashberg theory. The critical temperature of layered superconductors was calculated using this theory, and the influence of nonadiabaticity effects on the critical temperature was considered. In the calculation of the effect of Coulomb repulsion on the critical temperature, arbitrary thicknesses of conducting layers were also taken into account. In the same approach, expression for the plasmon spectrum of layered superconductors with arbitrary thicknesses of the conducting layers was obtained. In addition, Bardeen–Cooper–Schrieffer equations for layered superconductors were used for calculating the specific heat jump, which is smaller than in the isotropic case. The influence of fluctuations of the order parameter phase on the critical temperature of layered superconductors was studied using the Ginzburg–Landau functional for the free energy for layered superconductors. The results are shown to be in qualitative agreement with experimental data for cuprate superconductors and the recently discovered MgB_2 compound.

Acknowledgements
I thank F M Hashimzade, B M Askerov, and R R Guseinov for the useful discussions, and A M Hashimov for supporting the presented research. I am also grateful to the Abdus Salam ICTP for the hospitality during my stay as an associate member. This work was financially supported in part by the NATO reintegration grant 980766.

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